## 3,6-Diacetylmorphine

561-27-3 | DTXSID6046761

## Model Performance

| Model | Data |
|-------|------|

## Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

## Model Results

**Predicted value:** 1.04e-09 mmHg

**Global applicability domain:** Outside

**Local applicability domain index:** 3.34e-01

**Confidence level:** 5.06e-01

## Nearest Neighbors from the Training Set

Image not found
Pentane, 2,3,3-trimethyl-
**Measured:** 7.59e-10
**Predicted:** 29.7

Image not found
Fosthiazate
**Measured:** 3.30e-10
**Predicted:** 1.14e-05

Image not found
4-[Cyclopropyl(hydroxy)methylidene]-3,5-dioxocyclohexane-1-carboxylic acid
**Measured:** 5.63e-08
**Predicted:** 7.62e-09

Image not found
1,2,3,4,6-Pentachloronaphthalene
**Measured:** 8.70e-09
**Predicted:** 1.71e-06

Image not found
2,3',4-Trichlorodiphenyl ether
**Measured:** 1.20e-09
**Predicted:** 1.55e-04